Workshop on Software Productivity for Extreme-Scale Science (SWP4XS)

January 13-14, 2014
Hilton Washington DC / Rockville Hotel & Executive Meeting
Center in Rockville, MD

Organizing Committee: Hans Johansen (LBNL) and Lois Curfman McInnes (ANL), Co-Chairs
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Workshop Description:

The objective of this 1½-day workshop is to bring together computational scientists from academia, industry, and national laboratories to identify the major challenges of large-scale application software productivity on extreme-scale computing platforms. Large-scale development of new application codes and refactoring of existing scientific numerical software are emerging as major obstacles to the effective use of extreme-scale computing systems in modeling, simulating, and analyzing complex multiscale and multiphysics problems. Science goals include transitioning from qualitative to quantitative simulations that can predict experimental observations and inform high-impact policy and decision support. Software development is further complicated by the complexity of current petascale and anticipated exascale computing platforms, characterized by myriad novel architectural features, including millions of cores, simultaneous multithreading, vectorization, core heterogeneity, unconventional memory hierarchies, and new programming models. Given that major breakthroughs in many scientific domains across the Office of Science in DOE increasingly depend on complex modeling and simulation as well as integrated data analysis, understanding and addressing these software challenges are a major programmatic priority for ASCR and its scientific collaborators.

In this workshop, participants will assess the needs of computational science software in the age of extreme-scale multicore architectures, examine scientific software lifecycle and infrastructure requirements for large-scale code development efforts, and explore potential contributions and lessons learned that software engineering can bring to HPC software at scale. In addition, participants will identify short-term and long-term challenges of scientific software that must be addressed in order to significantly improve the productivity of emerging multicore-based extreme-scale computing systems through effective scientific software development processes and methodologies. The workshop will also explore scalable metrics for measuring the productivity of large scientific software systems.

Addressing these challenges in extreme-scale application software productivity is essential in order to fully exploit emerging hybrid architectures for scientific discovery. Moreover, because software is the practical means through which computational science collaboration occurs, this is a prime opportunity for synergistic work across the Office of Science, centered on partnerships between ASCR and its sister programs in DOE/SC, as well as activities in concert with NNSA and other DOE offices. The issues discussed during this workshop are expected to affect software productivity research in extreme-scale scientific applications and the mathematical and computer science software tools on which they depend.

An outcome of the workshop will be a report that articulates and prioritizes productivity challenges and recommends both short-term and long-term research directions for software productivity for extreme-scale science. The final report will be delivered to DOE by March 2014.